



chain nodes :  
1 16 17 18 19 20 21 22 23 24 25 26 32 33 40 41 42  
ring nodes :  
2 3 4 5 6 7 8 9 10 11 12 13 14 15 27 28 29 30 31 34 35 36 37 38 39  
chain bonds :  
1-2 10-11 12-16 13-17 14-18 18-19 19-20 20-21 20-22 22-23 23-24 23-25 25-26 26-27  
29-34 30-33 31-32 38-40 40-41 40-42  
ring bonds :  
2-3 2-7 3-4 4-5 5-6 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15 27-28  
27-31 28-29 29-30 30-31 34-35 34-37 35-36 36-39 37-38 38-39  
exact/norm bonds :  
1-2 2-7 3-4 5-6 6-10 7-8 8-9 9-10 10-11 11-12 11-15 12-13 12-16 13-14 13-17  
14-15 14-18 18-19 19-20 20-21 20-22 22-23 23-24 23-25 25-26 26-27 27-28 27-31  
28-29 29-30 29-34 30-31 30-33 31-32 34-35 34-37 35-36 36-39 37-38 38-39 38-40  
40-41 40-42  
normalized bonds :  
2-3 4-5 6-7

Match level :  
1:CLASS 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom  
32:CLASS 33:CLASS 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS  
42:CLASS